# METHOD AND APPARATUS FOR DETERMINING THE CHEMICAL STRUCTURE OF AN UNKNOWN SUBSTANCE

## BACKGROUND OF THE INVENTION

(1) Field of the Invention

The present invention relates to a method and apparatus for determining the chemical structure of an unknown substance by analysis of the spectral data of the unknown substance obtained from an analysis apparatus, particularly a C-13 nuclear magnetic resonance (below, C-13 NMR) apparatus.

(2) Description of the Prior Art

Up until now, analysis of the structure of an unknown substance has been effected using spectral data by the manual labor and intellectual, mental work of spectroscopists based on their personal experience and spectroscopic theory. This analysis work involves the comparison of the standard spectra of many amount of known substances, judging which features the unknown substance has in common with the spectra of the known substances, and thus deducing the composite elements of the molecular structure, i.e., the partial structures. This takes time and requires considerable experience in data analysis.

Recently, in the field of chemical structural analysis, the same procedures formerly carried out manually by human operators are being performed by computerized data searches, whereby up to tens of thousands of sets of standard spectral data of known substances are compared with the spectral data of the unknown substance so as to determine the chemical structure of the unknown substance.

However, in this conventional method, it is possible to identify an unknown substance as a known substance only when the standard spectral data of the known substance and the spectral data of the unknown substance are a perfect match. Consequently, there is a disadvantage in that no information can be obtained on an unknown substance having a spectrum not included in the standard spectral data. In other words, this conventional method unconditionally considers the position and intensity of the spectral signals in the standard spectral data of the known substances and the spectrum of the unknown substance as specific values and requires complete correspondence of the spectral signals as a condition for identification. Therefore, there is a shortcoming in that a difference in electron density due to a slight difference in molecular structure or a deviation in the numerical value due to an error in measurement makes identification of even a known substance impossible.

Further, up until now, the spectral data of known substances accumulated for C-13 NMR apparatuses covers only approximately 35,000 compounds—even with the most popular collection of standard spectral data compiled by the Satler Co. Almost no data on compounds being daily synthesized for the purpose of development and research of industrial products is contained therein, and for this reason, it is almost impossible, in particular, to determine the chemical structure of byproducts, etc. of synthetic reactions using the conventional method relying on a data search.

## SUMMARY OF THE INVENTION

The object of the present invention is, in consideration of the above-mentioned problems in the prior art, to provide a method and apparatus for determining the chemical structure of an unknown substance wherein the partial structures of known substances and the chemical shift values corresponding thereto are stored in advance in a memory apparatus and the chemical shift values and the spectral data of the unknown substance are used to assess, with a membership function, the possibility of the partial structures being contained in the unknown substance and, based on this concept, the partial structures contained in either an unknown substance or known substance can be automatically and quickly deduced and output from the C-13 NMR spectrum, from the results of which output spectroscopists and the like can easily determine the molecular structure.

In accordance with the present invention, there is provided an apparatus for determining the chemical structure of an unknown substance, comprising: a means for detecting spectral data of the unknown substance; a memory means for memorizing at least the chemical shift values corresponding to partial structures of known substances; a means for finding a point-assessment expressing the degree of possibility of partial structures being contained in the unknown substance based on the spectral data of the unknown substance and the data stored in the memory means; comparison means for judging whether the point-assessment is a predetermined threshold value or more; and an output means for displaying the partial structures with a large possibility of being contained in the unknown substance based on the output of the comparison means.

Also, in accordance with the present invention, there is provided a method for determining the chemical structure of an unknown substance comprising detecting spectral data of the unknown substance, finding a point-assessment expressing the degree of possibility of partial structures being contained in the unknown substance based on the spectral data and prememorized chemical shift values corresponding to the partial structures of known substances, judging whether the point-assessment is a predetermined threshold value or more; and finding and displaying the partial structures with a large possibility of being contained in the unknown substance based on the output of the judgement results.

## DESCRIPTION OF THE DRAWINGS

FIG. **1** is a block diagram showing the structure of an apparatus according to an embodiment of the present invention;

FIG. **2** is a flow chart showing the procedures for processing to determine the chemical structure of an unknown substance in the apparatus of FIG. **1**;

FIG. **3** is a graph explaining the method of calculation of the membership function;

FIG. **4** is a flowchart showing the details of the processing for calculating the point-assessment in FIG. **2**;

FIGS. **5A** and **5B** are graphs explaining in detail the method for calculating the point-assessment; and

FIG. **6** is a flowchart showing details of the processing for calculating the point-assessment showing the possibility of an aromatic ring substituent position isomer in FIG. **2**.